

PROTEIN STRUCTURE PRECTION USING THE ELASTIC NET ALGORITHM

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In this work we use the elastic net method applied to prediction of protein structure from their amino acid sequence. Initially we reproduce possible solutions of a classic optimization problem known as Salesman Travelling Problem (STP). We apply the strategy of Durbin-Willshaw elastic net (EN) method. To the STP the method can be associated with data base-derived potential and some experimental data, for example radius of giration, for predicting protein structure. We modify the potential function adding the hard core potential and in general we get a better root mean square (RMS) for protein structure predicted than literature.